5. COMPUTING ENVIRONMENT

5.1 High Performance Computing

The high performance computing resources in C-MMACS received a major boosting during the year 1997-98 with the addition of a multi-CPU server and midrange workstations. The Convex C3820 continues to serve the scientific community for their large scale computing requirements.

The most important enhancement of the year was the installation of SGI Origin 200 server, with most of the application software being made available on it which were earlier available on Convex C3820. The Origin server with four numbers of R10000 CPUs @180 MHz clock frequency is being upgraded with 1 GB main memory and 72 GB hard disk. After the upgradation, this server is expected to meet most of the midrange computing requirements of scientists from C-MMACS and other CSIR laboratories. Three numbers of R10000 based SGI O2 workstations were added to the computing environment enabling the scientists to perform visualisation of highly complex 3-dimensional modelling problems.

The Convex C3820 has successfully completed four years of excellent computing service and its total utilisation has exceeded 41,000 CPU hours. The system is being maintained in-house with technical advice and spares support from HP-Convex, Singapore which results in saving a considerable amount of foreign exchange.

5.2 Network and Hardware Enhancement

Upgradation of networks is a continuing requirement to keep pace with the increasing demand for network based computing and the availability of computer systems with powerful CPUs and faster network interfaces. In order to provide a good throughput to the end user and improve the efficiency of the total network, the C-MMACS LAN has gone through a major enhancement.

The LAN has been upgraded to a switch based network by procuring and installing Cisco switches with 10 & 100 Mbps ports. This enables desktops and workstations to have 10 Mbps switched connectivity to the full duplex fast ethernet (200 Mbps) backbone and 100 Mbps connectivity to the server. The FDDI network is interconnected through one of the switches. This upgraded network provides faster and collision free connectivity among the servers and workstations across the network.

Hardware enhancement becomes necessary as the computing requirements keep increasing with time. For faster visualisation of different modelling activities, the main memories of the SGI Indy front-end graphics workstations have been upgraded to 64 MB. For reliable storage and transfer of critical data, a 2.3 GB optical disk drive has been added to the LAN.

5.3 Internet and E-mail Service

Access to Internet and e-mail has now become essential for every one in an R & D centre as it facilitates scientists to exchange data and information with their counterparts anywhere in the globe instantly. This has resulted in the need for high speed communication links to the Internet. Keeping this in mind, the radio link between C-MMACS and ERNET gateway at STP was

Mathematical Libraries

DXML	Extended mathematical libraries	DEC
ELLPACK	Solvers for elliptic partial differential equations	CONVEX
IMSL	Comprehensive library for numerical and statistical analysis	SGI , INTEL
NUMERICAL RECIPES	Software for numerical analysis	SGI, INTEL
ITPACK	Iterative solvers for linear systems	CONVEX
LAPACK	Linear algebra	CONVEX
LINPACK	Linear system solver	CONVEX
NAG	Numerical and statistical analysis	CONVEX, SGI, INTEL
ODEPACK	Ordinary differential equation solvers	CONVEX
SPARSEPACK	Sparse linear system solvers	CONVEX
VECLIB	CONVEX vector libraries	CONVEX

Application Packages

Biology & Chemistry

AMBER 4	Modelling of peptides / nucleic acids / carbohydrates	CONVEX, SUN
GROMOS 95	Modelling of peptides / nucleic acids / carbohydrates	CONVEX
MOPAC 6	Molecular orbital calculations	CONVEX
PCMODEL	Molecular modelling	SGI
XPLOR	X-ray crystallographic and solution NMR structure determination	CONVEX

CAD/CAE

CAMAND	Computer aided modelling, analysis, numerical control, design and documentation	SGI
CFD-GEOM	Surface modelling and grid generation	SGI
SDRC I-DEAS	Solid modelling	SGI

Earth Sciences

BERNESE	GPS data processing	SUN
CCM 2	Community climate model	CONVEX
LOWTRAN 7	Atmospheric radiative transfer	CONVEX
MOM	Global ocean circular (Modular model)	CONVEX, DEC, SUN
TIDAL	Shallow water simulation and pollutant transport	CONVEX, INTEL

Fluid Flow, Heat and Mass Transfer

CFD-ACE	Computational fluid dynamics	CONVEX, SGI
NISA	Finite element fluid dynamics code	CONVEX, SGI
PHONENICS	Computational fluid dynamics	CONVEX, INTEL
PORFLOW	Porous media flow, heat and mass transfer	CONVEX, INTEL

Scientific Visualisation

AVS	Application visualisation system	CONVEX
CFD-VIEW	Graphics for CFD	SGI
GrADS	Graphical display for atmospheric and oceanic applications	SGI, DEC
NCAR Graphics	Advanced graphics display and mapping	SGI, SUN
TECPLOT	General purpose 3-D graphics	SGI, INTEL

Structural Mechanics

NISA	Finite element analysis	CONVEX, INTEL
SDRC I-DEAS	Finite element modelling	SGI

Miscellaneous		
ACRPLOT	General purpose plotting package	INTEL
CSS STATISTICA	Integrated statistical and graphics analysis	INTEL
MATLAB	Mathematical and symbolic computation	SGI, INTEL
NEXPERT	Expert system shell	INTEL
SPSS	Advanced statistical analysis	DEC
MACSYMA	Applied Mathematics software	SUN, INTEL
PDEase	Applied Mathematics software	SUN, INTEL
Graphics Libraries		
GKS		SGI
NAG Graphics		CONVEX, INTEL
PHIGS		SGI, DEC, SUN

enhanced to 64 Kbps and has enabled us to have faster access to the rest of the world on Internet and vice-versa. Due to the round-the-clock availability of necessary infrastructure, CSIR decided to host their official home page at C-MMACS and the same can be seen at the URL http://www.cmmacs.ernet.in/csir. In addition, the home page of National Aerospace Laboratories is also hosted on the C-MMACS webserver, and can be accessed through the URL http://www.cmmacs.ernet.in/nal.

C-MMACS has been chosen as one of the 15 laboratories under CSIR to have a VSAT connection as part of the upcoming CSIR NET. The installation of the VSAT equipment has already been completed and is expected to be operational once the transponder space becomes available in the INSAT series satellites. This will enable CSIR laboratories to come closer to C-MMACS for collaborative research work and provide an additional 64 Kbps connection to Internet through CSIR headquaters.

A new mail gateway and server has been installed and configured on a Compaq server with SCO OS. This has enabled direct delivery and receipt of mails to and from Internet and eliminated the need to go through a mail forwarding gateway of the ISP.

5.4 Software

Following the installation and commisioning of the Origin 200 server, many scientific software services have been migrated to it. A lot of public domain application software was installed on Origin 200 server in addition to Matlab, NISA, CFD-ACE, IMSL and Numerical Recipes. Macsyma and PDEase software have been procured and installed on Windows95 and Ultra Sparc platforms. The upgrade and transfer of Phoenics software from Convex to Origin 200 server is in process. The *table* above gives the list of software packages available along with a brief description and the platform on which they are installed.

5.5 Other Services

C-MMACS's high performance computing facility has been extensively used by scientists and researchers from various CSIR laboratories. Computing resources were provided to the students of Banga-lore University, Birla Institute of Technology and Science, Cochin University of Science and Technology, Madurai Kamaraj University, Mangalore University, Bharathiyar University and

Bharathidasan University to carry out their academic project work at C-MMACS.

5.6 Ongoing Enhancements

Following are the systems under procurement to strengthen the computing resources at C-MMACS:

1. SGI Origin 200 Webforce server.
2. 1 GB memory and 72 GB disk for Origin 200 server
3. 64 Kbps VSAT link through CSIRNET.

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